Strong interaction of correlated electrons with phonons: Exchange of phonon clouds by polarons

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Abstract

We investigate the interaction of strongly correlated electrons with phonons in the frame of the Hubbard-Holstein model. The electron-phonon interaction is considered to be strong and is an important parameter of the model besides the Coulomb repulsion of electrons and band filling. This interaction with the nondispersive optical phonons has been transformed to the problem of mobile polarons by using the canonical transformation of Lang and Firsov. We discuss in particular the case for which the on-site Coulomb repulsion is exactly cancelled by the phonon-mediated attractive interaction and suggest that polarons exchanging phonon clouds can lead to polaron pairing and superconductivity. It is then the frequency of the collective mode of phonon clouds being larger than the bare frequency, which determines the superconducting transition temperature.

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I. INTRODUCTION

Since the discovery of high-temperature superconductivity by Bednorz and Müller,[1] the Hubbard model and related models such as RVB and t-J have widely been used to discuss the physical properties of the normal and superconducting state.[2,3,4,5,6] However, a unanimous explanation of the origin of the condensate in high-temperature superconductors has not emerged so far. One of the unsolved questions is in how far can phonons be involved in the formation of the superconducting state. In experimental and theoretical works mostly the change of phonon frequencies and phonon life times associated with the superconducting transition were discussed. For example, the decrease of frequencies of Raman-active phonons at the transition[7] and observation of the isotope effect for the case of not optimally doped superconductors[8], as well as the observation of phonon-induced structure in the tunnel characteristics,[9] speak in favor of strong electron-phonon coupling in the cuprates.

The aim of the present paper is to gain further insight into the mutual influence of strong on-site Coulomb repulsion and strong electron-phonon interaction by using the single-band Hubbard-Holstein model and a recently developed diagrammatic approach.[10,11,12,13,14] For simplicity we consider coupling to dispersionless phonons only, although this might not be the most interesting case with respect to superconductivity. However, previous investigations[15,16,17] have shown that the Hubbard-Holstein model[18,19] constitutes a formidable problem of its own. Other authors have also intensively studied this model Hamiltonian.[20,21,22,23]

Because the interactions between electrons and electrons and phonons are strong, we include the Coulomb repulsion in the zero-order Hamiltonian and apply the canonical transformation of Lang and Firsov[24] in order to eliminate the linear electron-phonon interaction. In the strong electron-phonon coupling limit the resulting Hamiltonian of hopping polarons (i.e., hopping electrons surrounded by clouds of phonons) can lead to an attractive interaction among electrons being mediated by the phonons. In this limit the chemical potential, on-site Coulomb energy as well as the frequency of the collective mode of phonon clouds (which is much larger than the bare frequency of the Einstein oscillators) are strongly renormalized[17,25,26] affecting the dynamical properties of the polarons and the character of the superconducting transition. This will be discussed by assuming that renormalized on-site Coulomb repulsion and attractive electron-electron interaction completely cancel each

other. We suggest that the resulting superconducting state with polaronic Cooper pairs is mediated by the exchange of phonon clouds during the hopping processes of the electrons.

II. THEORETICAL APPROACH

A. The Lang-Firsov transformation of the Hubbard-Holstein model

The initial Hamiltonian of correlated electrons coupled to optical phonons with bare frequency ω_0 is given by

$$\mathcal{H} = \mathcal{H}_e + \mathcal{H}_{ph}^0 + \mathcal{H}_{e-ph}, \tag{1}$$

$$\mathcal{H}_e = \sum_{ij\sigma} \{t(j-i) - \epsilon_0\,\delta_{ij}\}\, a_{j\sigma}^\dagger a_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{2}$$

$$\mathcal{H}_{ph}^0 = \sum_i \hbar\omega_0 \left(b_i^\dagger b_i + \tfrac{1}{2} \right), \qquad \mathcal{H}_{e-ph} = g \sum_i n_i q_i, \tag{3}$$

$$n_i = \sum_\sigma n_{i\sigma}, \quad n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}, \quad q_i = \frac{1}{\sqrt{2}} \left(b_i + b_i^\dagger \right). \tag{4}$$

Here $a_{i\sigma}^\dagger$ ($a_{i\sigma}$) and $b_i^\dagger$ (b_i) are creation (annihilation) operators of electrons and phonons, respectively; i refers to the lattice site and σ to the spin; q_i is the phonon coordinate and g the electron-phonon interaction constant; $\epsilon_0 = \bar{\epsilon}_0 - \mu$ with local energy $\bar{\epsilon}_0$ and chemical potential μ; U the on-site Coulomb repulsion; $t(j-i)$ is the two-center transfer integral. The Fourier representation of $t(j-i)$ is connected to the tight-binding dispersion $\varepsilon(\mathbf{k})$ of the bare electrons,

$$t(j-i) = \frac{1}{N} \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) \exp\{-i\mathbf{k}(\mathbf{R}_j - \mathbf{R}_i)\},$$

with band width W. The energy scale of this model is fixed by the parameters W, U, g and $\hbar\omega_0$. As an additional parameter we have the band filling.

After applying the Lang-Firsov transformation[24]

$$\mathcal{H}_p = e^S \mathcal{H} e^{-S}, \quad c_{i\sigma} = e^S a_{i\sigma} e^{-S}, \quad c_{i\sigma}^\dagger = e^S a_{i\sigma} e^{-S} \tag{5}$$

with

$$S = -i\bar{g} \sum_i n_i p_i, \quad \bar{g} = \frac{g}{\hbar\omega_0}, \quad p_i = \frac{i}{\sqrt{2}} \left(b_i^\dagger - b_i \right), \tag{6}$$

3

where p_i is the phonon momentum and $\bar{g}$ the dimensionless interaction constant, the polaron Hamiltonian is obtained as

$$\mathcal{H}_p = \mathcal{H}_p^0 + \mathcal{H}_{ph}^0 + \mathcal{H}_{int}, \tag{7}$$

$$\mathcal{H}_p^0 = \sum_i \mathcal{H}_{ip}^0, \quad \mathcal{H}_{ip}^0 = \epsilon \sum_\sigma n_{i\sigma} + \bar{U} n_{i\uparrow} n_{i\downarrow}, \tag{8}$$

$$\mathcal{H}_{int} = \sum_{i,j,\sigma} t(j-i) c_{j\sigma}^\dagger c_{i\sigma}, \tag{9}$$

$$c_{i\sigma}^\dagger = a_{i\sigma}^\dagger e^{-i\bar{g}p_i}, \quad c_{i\sigma} = a_{i\sigma} e^{i\bar{g}p_i}, \tag{10}$$

$$\epsilon = \bar{\epsilon}_0 - \bar{\mu}, \quad \bar{\mu} = \mu + \alpha\hbar\omega_0, \quad \bar{U} = U - 2\alpha\hbar\omega_0, \quad \alpha = \tfrac{1}{2}\bar{g}^2. \tag{11}$$

In order to derive the polaron Hamiltonian it was necessary to include the shift of the phonon coordinate q_i of the form $e^S q_i e^{-S} = q_i - \bar{g} n_i$ which is responsible for the elimination of the linear electron-phonon interaction. The polaron Hamiltonian is by nature a polaron-phonon operator, i.e., the creation operator $c_{i\sigma}^\dagger$ and destruction operator $c_{i\sigma}$ in $\mathcal{H}_p$ should be interpreted as creation and destruction operators of polarons (electrons dressed with the displacements of the ions) which couple dynamically to the momentum of the optical phonon. In zero-order approximation (omitting $\mathcal{H}_{int}$) polarons and phonons are localized with strongly renormalized chemical potential $\bar{\mu}$ and on-site Coulomb interaction $\bar{U}$. The operator $\mathcal{H}_{int}$ describes the tunneling of polarons between the lattice sites, i.e., tunneling of electrons surrounded by clouds of phonons.

B. Expansion about the atomic limit

The problem is now to deal properly with the impact of electronic correlations on the polaron problem. This can be done best by using Green's functions provided one finds a key to deal with the spin and charge degrees of freedom. For the general case when $\bar{U}$ is different from zero, the Coulomb interaction has to be included in the zero-order Hamiltonian. As a consequence conventional perturbation theory of quantum statistical mechanics is not an adequate tool because it relies on the expansion of the partition function about the noninteracting state (use of traditional Wick's theorem and conventional Feynman diagrams). Similar is the situation for composite particles like polarons, $c_{i\sigma} = a_{i\sigma} \exp(i\bar{g}p_i)$, involving operators for the electron and phonon subsystem.

It was Hubbard[27] who proposed a graphical expansion for correlated electrons about the atomic limit in powers of the hopping integrals. This diagrammatic approach was reformulated in a systematic way for the single-band Hubbard model by Slobodyan and Stasyuk,[28] and, independently, by Zaitsev[29] and further developed by Izyumov.[30] In these approaches the complicated algebraical structure of projection or Hubbard operators was used. Therefore, it appeared to be more appropriate to develop a diagrammatic technique which uses more simple creation and annihilation operators for electrons at all intermediate stages of the theory (for details see Ref. 10,11). In the latter approach the averages of chronological products of interactions are reduced to n-particle Matsubara Green's functions of the atomic system. These functions can be factorized into independent local averages by using a generalization of Wick's theorem (GWT), which takes into account strong local correlations (details are given in Ref. 10,11,25). The application of GWT yields new irreducible on-site many-particle Green's functions or Kubo cumulants. These new functions contain all local spin and charge fluctuations. The analogical linked-cluster expansion for the Hubbard model around the atomic limit was recently reformulated by Metzner.[31]

C. Averages of phonon operators

We define the temperature Green's function for the polarons in (7) in the interaction representation by

$$\mathcal{G}(\mathbf{x}, \sigma, \tau | \mathbf{x}', \sigma', \tau') = -\langle T\, c_{\mathbf{x}\sigma}(\tau)\, \bar{c}_{\mathbf{x}'\sigma'}(\tau')\, U(\beta) \rangle_0^c, \tag{12}$$

with

$$c_{\mathbf{x}\sigma}(\tau) = e^{\mathcal{H}^0 \tau} c_{\mathbf{x}\sigma} e^{-\mathcal{H}^0 \tau}, \quad \bar{c}_{\mathbf{x}\sigma}(\tau) = e^{\mathcal{H}^0 \tau} c_{\mathbf{x}\sigma}^\dagger e^{-\mathcal{H}^0 \tau},$$

with $\mathcal{H}^0 = \mathcal{H}_p^0 + \mathcal{H}_{ph}^0$ and evolution operator given by

$$U(\beta) = T \exp\left(- \int_0^\beta d\tau\, H_{int}(\tau)\right), \tag{13}$$

and where $\mathbf{x}, \mathbf{x}'$ are the site indices and τ, τ' stand for the imaginary time with $0 < \tau < \beta$; T is the time ordering operator and β the inverse temperature. The statistical average $\langle \ldots \rangle_0^c$ is evaluated with respect to the zero-order density matrix of the grand-canonical ensemble of the localized polarons and phonons

$$\frac{e^{-\beta \mathcal{H}^0}}{\mathrm{Tr}\, e^{-\beta \mathcal{H}^0}} = \prod_i \frac{e^{-\beta \mathcal{H}_{i\,p}^0}}{\mathrm{Tr}\, e^{-\beta \mathcal{H}_{i\,p}^0}} \frac{e^{-\beta \mathcal{H}_{i\,ph}^0}}{\mathrm{Tr}\, e^{-\beta \mathcal{H}_{i\,ph}^0}} \tag{14}$$

The upper index 'c' in (13) means that only connected diagrams must be taken into account. The density matrix (14) is factorized with respect to the lattice sites. The phonon part is easily diagonalized by using the free phonon operators, b_i and $b_i^\dagger$, while the on-site polaron Hamiltonian contains the polaron-polaron interaction which is proportional to the renormalized parameter $\bar{U}$, which only can be diagonalized by using Hubbard operators.[18] At this stage no special assumption is made about the quantity $\bar{U}$ and its sign and we will set up the equations of motion for the dynamical quantities for this general case. However, a detailed inspection of the equations will only be undertaken for the special case $\bar{U} = 0$.

Wick's theorem of weak-coupling quantum field theory can be used when evaluating statistical averages of phonon operators like, for example, the propagator for the phonon cloud,

$$
\begin{aligned}
\Phi(\tau_1|\tau_2) = \Phi(\tau_1 - \tau_2) &\equiv \langle T \exp\{i\bar{g}\left[p(\tau_1) - p(\tau_2)\right]\}\rangle_0 \\
&= \exp\left(-\tfrac{1}{2}\bar{g}^2\langle T\left[p(\tau_1) - p(\tau_2)\right]^2\rangle_0\right) \\
&= \exp\left(-\sigma(\beta) + \sigma(|\tau_1 - \tau_2|)\right),
\end{aligned}
\tag{15}
$$

$$
\begin{aligned}
\Phi(\tau_1, \tau_2|\tau_3, \tau_4) &\equiv \langle\, T\, \exp\{i\bar{g}\left[p(\tau_1) + p(\tau_2) - p(\tau_3) - p(\tau_4)\right]\}\rangle_0 = \\
&= \exp\left(-\tfrac{1}{2}\bar{g}^2\langle T\left[p(\tau_1) + p(\tau_2) - p(\tau_3) - p(\tau_4)\right]^2\rangle_0\right) \\
&= \exp\{\sigma(|\tau_1 - \tau_3|) + \sigma(|\tau_1 - \tau_4|) + \sigma(|\tau_2 - \tau_3|) \\
&+\ \sigma(|\tau_2 - \tau_4|) - \sigma(|\tau_1 - \tau_2|) - \sigma(|\tau_3 - \tau_4|) \\
&-\ 2\sigma(\beta)\},
\end{aligned}
\tag{16}
$$

where

$$
\begin{aligned}
\sigma\left(|\tau_1 - \tau_2|\right) &= \bar{g}^2\langle T\, p(\tau_1)p(\tau_2)\rangle_0 \\
&= \alpha \frac{\cosh\left(\hbar\omega_0\left\{\dfrac{\beta}{2} - |\tau_1 - \tau_2|\right\}\right)}{\sinh\left(\dfrac{\beta\hbar\omega_0}{2}\right)}.
\end{aligned}
\tag{17}
$$

We now have to discuss the problem of how to calculate chronological averages of combinations of polaron operators. Here we will make use of the above mentioned new diagram technique and the GWT.[10,11] This approach has many-particle on-site irreducible Green's functions as main element of the diagrams.

6

III. POLARON AND PHONON GREEN'S FUNCTIONS

In zero-order approximation the one-polaron Green's function is of the form

$$
\begin{aligned}
\mathcal{G}_p^0(x|x') &= -\langle T\, c_{\mathbf{x}\sigma}(\tau)\bar{c}_{\mathbf{x}'\sigma'}(\tau')\rangle_0 \\
&= -\langle T\, a_{\mathbf{x}\sigma}(\tau)\bar{a}_{\mathbf{x}'\sigma'}(\tau')\rangle_0 \Phi(\tau|\tau') \\
&= \mathcal{G}^{(0)}(x|x')\,\Phi(\tau|\tau'),
\end{aligned}
\tag{18}
$$

with $x = (\mathbf{x}, \sigma, \tau)$. The simplest new element of the diagram technique is the two-particle irreducible Green's function or Kubo cumulant, which is equal to

$$
\begin{aligned}
\mathcal{G}_2^{(0)\,ir}(x_1, x_2|x_3, x_4) ={}& \delta_{\mathbf{x}_1,\mathbf{x}_2}\delta_{\mathbf{x}_1,\mathbf{x}_3}\delta_{\mathbf{x}_1,\mathbf{x}_4} \\
&\times \mathcal{G}_2^{(0)\,ir}(\sigma_1, \tau_1; \sigma_2, \tau_2|\sigma_3, \tau_3; \sigma_4, \tau_4),
\end{aligned}
\tag{19}
$$

where

$$
\begin{aligned}
\mathcal{G}_2^{(0)\,ir}&(\sigma_1, \tau_1; \sigma_2, \tau_2|\sigma_3, \tau_3; \sigma_4, \tau_4) \\
={}& \langle T\, c_{\sigma_1}(\tau_1)\, c_{\sigma_2}(\tau_2)\bar{c}_{\sigma_3}(\tau_3)\,\bar{c}_{\sigma_4}(\tau_4)\rangle_0 \\
&- \langle T\, c_{\sigma_1}(\tau_1)\,\bar{c}_{\sigma_4}(\tau_4)\rangle_0\langle T\, c_{\sigma_2}(\tau_2)\,\bar{c}_{\sigma_3}(\tau_3)\rangle_0 \\
&+ \langle T\, c_{\sigma_1}(\tau_1)\,\bar{c}_{\sigma_3}(\tau_3)\rangle_0\langle T\, c_{\sigma_2}(\tau_2)\,\bar{c}_{\sigma_4}(\tau_4)\rangle_0.
\end{aligned}
\tag{20}
$$

The first term on the right-hand side of Eq. (21) is of the form

$$
\begin{aligned}
\langle T\, c_{\sigma_1}(\tau_1)&\, c_{\sigma_2}(\tau_2)\,\bar{c}_{\sigma_3}(\tau_3)\,\bar{c}_{\sigma_4}(\tau_4)\rangle_0 \\
&= \langle T\, a_{\sigma_1}(\tau_1)\, a_{\sigma_2}(\tau_2)\,\bar{a}_{\sigma_3}(\tau_3)\,\bar{a}_{\sigma_4}(\tau_4)\rangle_0\,\Phi(\tau_1\tau_2|\tau_3\tau_4)
\end{aligned}
\tag{21}
$$

When the number of polaron operators increases more complicated irreducible Green's Functions like $\mathcal{G}_n^{(0)ir}(x_1 \ldots x_n|x'_1 \ldots x'_n)$ with $n \geq 3$ and all possible terms of their products will appear. The sum of all *strongly connected diagrams* (i.e., those which cannot be divided into two parts by cutting a single hopping line) containing all kinds of irreducible Green's functions in the perturbation expansion of the evolution operator, defines the special function $Z(x|x')$ (for details see Ref. 10,11). This function contains all contributions from charge and spin fluctuations. It allows us, together with the mass operator which is in our case the hopping matrix element, to formulate a Dyson-type of equation for the one-polaron Green's function,[10,11,12,13,14]

$$
\mathcal{G}(x|x') = \Lambda(x|x') + \sum_{1,2} \Lambda(x|1)t(1-2)\mathcal{G}(2|x'),
\tag{22}
$$

where

$$\Lambda(x|x') = \mathcal{G}_p^{(0)}(x|x') + Z(x|x'), \tag{23}$$

$$t(x - x') = \delta_{\sigma,\sigma'}\delta(\tau - \tau')\,t(\mathbf{x} - \mathbf{x}'). \tag{24}$$

Here x stands again for $\mathbf{x}, \sigma, \tau$ and the sum is over the discrete indices including the integration over τ. Using the Fourier representation for these quantities,

$$\mathcal{G}(\mathbf{x}|\tau) = \frac{1}{N}\sum_{\mathbf{k}}\frac{1}{\beta}\sum_{\omega_n}e^{-i\mathbf{k}\mathbf{x}-i\omega_n\tau}\mathcal{G}_\sigma(\mathbf{k}|i\omega_n),$$

$$\Lambda(\mathbf{x}|\tau) = \frac{1}{N}\sum_{\mathbf{k}}\frac{1}{\beta}\sum_{\omega_n}e^{-i\mathbf{k}\mathbf{x}-i\omega_n\tau}\Lambda_\sigma(\mathbf{k}|i\omega_n),$$

$$\mathcal{G}(\mathbf{x}|i\omega_n) = \frac{1}{2}\int_{-\beta}^{+\beta}d\tau\,e^{i\omega_n\tau}\mathcal{G}_\sigma(\mathbf{x}|\tau),$$

$$\Lambda(\mathbf{x}|i\omega_n) = \frac{1}{2}\int_{-\beta}^{+\beta}d\tau\,e^{i\omega_n\tau}\Lambda_\sigma(\mathbf{x}|\tau), \tag{25}$$

gives us the following form of the Dyson equation for the renormalized one-polaron Green's function,

$$\mathcal{G}_\sigma(\mathbf{k}|i\omega_n) = \frac{\Lambda_\sigma(\mathbf{k})}{1 - \varepsilon(\mathbf{k})\,\Lambda(\mathbf{k}|i\omega_n)} \tag{26}$$

Here ω_n stands for the odd Matsubara frequency, $\omega_n = (2n+1)\,\pi/\beta$.

For further discussion of $\mathcal{G}_\sigma(k|i\omega)$ we need the Fourier representation of the zero-order one-polaron Green's function $\mathcal{G}_p^{(0)}$ defined in (18). In order to facilitate the investigation we have evaluated the propagator of the phonon cloud (16) in the strong-coupling limit $\alpha \gg 1$,[15,16,26]

$$\Phi(\tau) = \frac{1}{\beta}\sum_{\Omega_n}e^{-i\Omega_n(\tau)}\bar{\Phi}(i\Omega_n), \tag{27}$$

$$\bar{\Phi}(i\Omega_n) = \frac{e^{-\sigma(\beta)}}{2}\int_{-\beta}^{\beta}d\tau\,e^{i\Omega_n\tau+\sigma(|\tau|)} \tag{28}$$

with $\Omega_n = 2n\pi/\beta$. In order to find $\bar{\Phi}(i\Omega_n)$ we use the Laplace approximation[32] for the integral (28) which contains an exponential function with the parameter α. In the strong-coupling limit $\alpha \gg 1$ we have obtained

$$\bar{\Phi}(i\Omega n) \approx \frac{2\omega_c}{\Omega_n^2 + \omega_c^2}, \quad \omega_c = \hbar\alpha\omega_0 = \hbar\frac{g^2}{2\hbar\omega_0}. \tag{29}$$

8

This term is the harmonic propagator of the collective mode of phonons belonging to the polaron clouds. There are further terms describing anharmonic deviations. For $\alpha \gg 1$ these terms will be omitted since they are smaller compared to the harmonic contribution. We obtain then for the Fourier representation of the phonon correlation function by making use of the Laplace approximation[32] and

$$\Phi(\tau_1, \tau_2 | \tau_3, \tau_4) = \frac{1}{\beta^4} \sum_{\Omega_1 \ldots \Omega_4} \bar{\Phi}(i\Omega_1, i\Omega_2 | i\Omega_3, i\Omega_4)\, e^{-i\Omega_1\tau_1 - i\Omega_2\tau_2 + i\Omega_3\tau_3 + i\Omega_4\tau_4}, \tag{30}$$

$$\bar{\Phi}(i\Omega_1, i\Omega_2 | i\Omega_3, i\Omega_4) = \int_0^\beta \ldots \int_0^\beta d\tau_1 \ldots d\tau_4\, e^{i\Omega_1\tau_1 + i\Omega_2\tau_2 - i\Omega_3\tau_3 - i\Omega_4\tau_4}, \tag{31}$$

the result

$$\bar{\Phi}(i\Omega_1, i\Omega_2 | i\Omega_3, i\Omega_4) \simeq [\delta_{\Omega_1,\Omega_3}\delta_{\Omega_2,\Omega_4} + \delta_{\Omega_1,\Omega_4}\delta_{\Omega_2,\Omega_3}]\, \bar{\Phi}(i\Omega_1)\, \bar{\Phi}(i\Omega_2), \tag{32}$$

which corresponds to

$$\Phi(\tau_1, \tau_2 | \tau_3, \tau_4) \simeq \Phi(\tau_1 | \tau_3)\, \Phi(\tau_2 | \tau_4) + \Phi(\tau_1 | \tau_4)\, \Phi(\tau_2 | \tau_3). \tag{33}$$

This means that we keep in the following only the free collective oscillations of the phonon clouds (29) which surround the polarons and use the Hartree-Fock approximation (32) and (33) for their two-particle correlation functions. In particular we will investigate the influence of absorption and emission of this collective mode (by the polarons) on the superconducting phase transition.

By using the harmonic mode (29) the Fourier representation of the local polaron Green's function

$$\bar{\mathcal{G}}_{p\sigma}^{(0)}(i\omega_n) = \frac{1}{2} \int_{-\beta}^\beta d\tau\, e^{i\omega_n\tau} \bar{\mathcal{G}}_{p\sigma}^{(0)}(\tau) \tag{34}$$

is equal to

$$\begin{aligned}
\bar{\mathcal{G}}_{p\sigma}^{(0)}(i\omega_n) \simeq \frac{1}{Z_0} \Bigg(&\frac{e^{-\beta E_0} + \bar{N}(\omega_c)(e^{-\beta E_0} + e^{-\beta E_\sigma})}{i\omega_n + E_0 - E_\sigma - \omega_c} \\
&+ \frac{e^{-\beta E_\sigma} + \bar{N}(\omega_c)(e^{-\beta E_0} + e^{-\beta E_\sigma})}{i\omega_n + E_0 - E_\sigma + \omega_c} \\
&+ \frac{e^{-\beta E_{-\sigma}} + \bar{N}(\omega_c)(e^{-\beta E_\sigma} + e^{-\beta E_2})}{i\omega_n + E_{-\sigma} - E_2 - \omega_c} \\
&+ \frac{e^{-\beta E_2} + \bar{N}(\omega_c)(e^{-\beta E_\sigma} + e^{-\beta E_2})}{i\omega_n + E_{-\sigma} - E_2 + \omega_c} \Bigg),
\end{aligned} \tag{35}$$

where

$$Z_0 = 1 + e^{-\beta E_\sigma} + e^{-\beta E_{-\sigma}} + e^{-\beta E_2}, \tag{36a}$$

$$E_0 = 0, \quad E_{\pm\sigma} = \epsilon, \quad E_2 = \bar{U} + 2\epsilon, \tag{36b}$$

$$\bar{n}(\epsilon) = \left(e^{\beta\epsilon} + 1\right)^{-1}, \quad \bar{N}(\omega_c) = \left(e^{\beta\omega_c} - 1\right)^{-1}. \tag{37}$$

Equation (35) shows that the on-site transition energies of the polarons are changed by the collective-mode energy $\pm\omega_c$ of the phonon clouds. The delocalization of the polarons due to their hopping between the lattice sites causes the broadening of the polaron energy levels. Equation (35) can be further simplified for the case of small on-site interaction energy $\bar{U}$ of polarons. For $\bar{U} = 0$ we obtain

$$\begin{aligned}
\bar{\mathcal{G}}_{p\sigma}^{(0)}(i\omega_n|\epsilon) &= \frac{\bar{N}(\omega_c) + 1 - \bar{n}(\epsilon)}{i\omega_n - \epsilon - \omega_c} + \frac{\bar{N}(\omega_c) + \bar{n}(\epsilon)}{i\omega_n - \epsilon + \omega_c} \\
&= \frac{(i\omega_n - \epsilon)\coth(\beta\omega_c/2) + \omega_c\tanh(\beta\epsilon/2)}{(i\omega_n - \epsilon)^2 - \omega_c^2}.
\end{aligned} \tag{38}$$

This function has the antisymmetric property

$$\bar{\mathcal{G}}_{p\sigma}^{(0)}(-i\omega_n| - \epsilon) = -\bar{\mathcal{G}}_{p\sigma}^{(0)}(i\omega_n|\epsilon) \tag{39}$$

which holds also for the renormalized polaron quantities,

$$\begin{aligned}
\Lambda_\sigma(-\mathbf{k}, -i\omega_n| - \epsilon) &= -\Lambda_\sigma(\mathbf{k}, i\omega_n|\epsilon), \\
\mathcal{G}_\sigma(-\mathbf{k}, -i\omega_n| - \epsilon) &= -\mathcal{G}_\sigma(\mathbf{k}, i\omega_n|\epsilon).
\end{aligned} \tag{40}$$

When taking $\bar{U} \simeq 0$ we assume that the strong on-site Coulomb repulsion of polarons can be canceled by the attraction induced by the strong electron-phonon interaction. We consider this as a model case which allows to discuss in a transparent manner the polarons exchanging phonon clouds during hopping between the lattice sites.

IV.   TWO-PARTICLE IRREDUCIBLE CORRELATION FUNCTIONS

In the following we discuss the influence of strong electron-phonon interaction on the two-particle irreducible Green's function. For $\bar{U} = 0$ the electronic correlation function in

(22) is equal to

$$\langle T\, a_{\sigma_1}(\tau_1)\, a_{\sigma_2}(\tau_2)\, \bar{a}_{\sigma_3}(\tau_3)\, \bar{a}_{\sigma_4}(\tau_4)\rangle_0$$

$$= \langle T\, a_{\sigma_1}(\tau_1)\bar{a}_{\sigma_4}(\tau_4)\rangle_0 \langle T\, a_{\sigma_2}(\tau_2)\bar{a}_{\sigma_3}(\tau_3)\rangle_0$$

$$- \langle T\, a_{\sigma_1}(\tau_1)\bar{a}_{\sigma_3}(\tau_3)\rangle_0 \langle T\, a_{\sigma_2}(\tau_2)\bar{a}_{\sigma_4}(\tau_4)\rangle_0 \tag{41}$$

because usual Wick's theorem works now. Making use of (33) we obtain for the two-particle irreducible Green's function (21) the relation,

$$\mathcal{G}_2^{(0)\,ir}(\sigma_1,\tau_1;\sigma_2,\tau_2|\sigma_3,\tau_3;\sigma_4\tau_4)$$

$$= \delta_{\sigma_1,\sigma_4}\delta_{\sigma_2,\sigma_3}\, \mathcal{G}_{\sigma_1}^{(0)}(\tau_1-\tau_4)\, \mathcal{G}_{\sigma_2}^{(0)}(\tau_2-\tau_3)\, \Phi(\tau_1-\tau_3)\, \Phi(\tau_2-\tau_4)$$

$$- \delta_{\sigma_1,\sigma_3}\delta_{\sigma_2,\sigma_4}\, \mathcal{G}_{\sigma_1}^{(0)}(\tau_1-\tau_3)\, \mathcal{G}_{\sigma_2}^{(0)}(\tau_2-\tau_4)\, \Phi(\tau_1-\tau_4)\, \Phi(\tau_2-\tau_3). \tag{42}$$

In the absence of exchange of phonon clouds by the polarons this quantity has to be zero. Indeed, if during the time of propagation of two polarons the electrons keep their initial phonon clouds, then the irreducible two-polaron Green's function (21) will vanish for the case $\bar{U}=0$. But because two electrons can be exchanged (independently of the exchange of phonon clouds) we obtain new contributions corresponding to two polarons with exchanged phonon clouds. Alternatively we may say that, in the case $\bar{U}=0$, Wick's theorem works separately for free electrons and free phonons; however, it does not apply for polarons as composite particles. Hence their cumulants do not vanish.

The Fourier representation of (42),

$$\mathcal{G}_2^{(0)\,ir}(\sigma_1,i\omega_1;\sigma_2,i\omega_2|\sigma_3,i\omega_3;\sigma_4,i\omega_4)$$

$$= \int_0^\beta \ldots \int_0^\beta d\tau_1 \ldots d\tau_4\, \mathcal{G}_2^{(0)\,ir}(\sigma_1,\tau_1;\sigma_2,\tau_2|\sigma_3,\tau_3;\sigma_4,\tau_4)\, e^{i\omega_1\tau_1+i\omega_2\tau_2-i\omega_3\tau_3-i\omega_4\tau_4}, \tag{43}$$

has the form

$$\mathcal{G}_2^{(0)\,ir}(\sigma_1,i\omega_1;\sigma_2,i\omega_2|\sigma_3,i\omega_3;\sigma_4,i\omega_4)$$

$$= \beta\, \delta_{\omega_1+\omega_2,\omega_3+\omega_4}\, \bar{\mathcal{G}}_2^{(0)\,ir}(\sigma_1,i\omega_1;\sigma_2,i\omega_2|\sigma_3,i\omega_3;\sigma_4,i\omega_4)$$

$$= \beta\, \delta_{\omega_1+\omega_2,\omega_3+\omega_4}\, \{\delta_{\sigma_1,\sigma_4}\, \delta_{\sigma_2,\sigma_3}\, A_{\sigma_1\sigma_2}(\sigma_1,i\omega_1;\sigma_2,i\omega_2|\sigma_2,i\omega_3;\sigma_1,i\omega_4)$$

$$- \delta_{\sigma_1,\sigma_3}\, \delta_{\sigma_2,\sigma_4}\, A_{\sigma_1\sigma_2}(\sigma_1,i\omega_1;\sigma_2,i\omega_2|\sigma_1,i\omega_4;\sigma_2,i\omega_3)\}, \tag{44}$$

where

$$A_{\sigma_1\sigma_2}(\sigma_1, i\omega_1; \sigma_2, i\omega_2 | \sigma_2, i\omega_3; \sigma_1, i\omega_4)$$

$$= \frac{1}{\beta} \sum_{\Omega} \frac{(2\omega_c)^2}{[i\omega_1 - \Omega - \epsilon][i\omega_3 - \Omega - \epsilon][\Omega^2 + \omega_c^2][(\Omega + \Omega_1)^2 + \omega_c^2]} \tag{45}$$

with $\Omega_1 = \omega_2 - \omega_3$. The summation leads to

$$A_{\sigma_1\sigma_2}(\sigma_1, i\omega_1; \sigma_2, i\omega_2 | \sigma_2, i\omega_3; \sigma_1, i\omega_4) = 2(\omega_c)^2$$

$$\times \left\{ \frac{\tanh(\beta\epsilon/2)\,[i\omega_1 + i\omega_2 - 2\epsilon][2\omega_c^2 - (i\omega_1 - \epsilon)(i\omega_4 - \epsilon) - (i\omega_2 - \epsilon)(i\omega_3 - \epsilon)]}{[(i\omega_1 - \epsilon)^2 - \omega_c^2][(i\omega_2 - \epsilon)^2 - \omega_c^2][(i\omega_3 - \epsilon)^2 - \omega_c^2][(i\omega_4 - \epsilon)^2 - \omega_c^2]} \right.$$

$$- \frac{2\omega_c[i\omega_1 + i\omega_2 - 2\epsilon]^2 \coth(\beta\omega_c/2)\,[2\omega_c^2 - (i\omega_1 - \epsilon)(i\omega_3 - \epsilon) - (i\omega_2 - \epsilon)(i\omega_4 - \epsilon)]}{[(i\Omega_1)^2 - (2\omega_c)^2][(i\omega_1 - \epsilon)^2 - \omega_c^2][(i\omega_2 - \epsilon)^2 - \omega_c^2][(i\omega_3 - \epsilon)^2 - \omega_c^2][(i\omega_4 - \epsilon)^2 - \omega_c^2]}$$

$$- \frac{\coth(\beta\omega_c/2)}{\omega_c[(i\Omega_1)^2 - (2\omega_c)^2]} \left[\frac{(i\omega_1 - \epsilon)(i\omega_3 - \epsilon) + 3\omega_c^2}{[(i\omega_1 - \epsilon)^2 - \omega_c^2][(i\omega_3 - \epsilon)^2 - \omega_c^2]} \right.$$

$$+ \left. \left. \frac{(i\omega_2 - \epsilon)(i\omega_4 - \epsilon) + 3\omega_c^2}{[(i\omega_2 - \epsilon)^2 - \omega_c^2][(i\omega_4 - \epsilon)^2 - \omega_c^2]} \right] \right\} \tag{46}$$

The function $A_{\sigma_1\sigma_2}$ contains the contributions to the two-particles on-site Green's function from the different spin channels. The spin structure in Eq. (44) is due to the conversation law for the spins of the polarons.

V. SUPERCONDUCTING PHASE TRANSITION

In the following we check whether the polaronic system may have a superconducting instability in the absence of a direct attractive interaction for the polarons, i.e., for $\bar{U} = 0$. In this case the attraction is only brought about dynamically by polarons exchanging phonon clouds. With respect to superconductivity we need in addition to the normal state Green's function (13) the anomalous propagators.[33] For simplicity we limit the discussion to s-wave superconductivity as in previous investigations of superconducting instabilities in the Hubbard model[13,14] and Hubbard-Holstein model in the strong-coupling limit, $\alpha \gg 1$.[26]

For a description of the superconducting state we need the three irreducible functions Λ_σ, $Y_{\sigma,-\sigma}$ and $\bar{Y}_{-\sigma,\sigma}$ which represent infinite sums of diagrams containing irreducible many-particle Green's functions. In order to obtain a close set of equations we will restrict ourselves to a class of rather simple contributions which, however, contain the most important charge, spin and pairing correlations; for details see Ref. 26. This class of diagrams is obtained by

neglecting contributions for which the Fourier representation of the superconducting order parameters, $Y_{\sigma,-\sigma}$ and $\bar{Y}_{-\sigma,\sigma}$, depend on the polaron momentum $\mathbf{k}$. In this approximation $Y_{\sigma,-\sigma}$ has to be obtained from

$$Y_{\sigma,-\sigma}(i\omega) = -\frac{1}{\beta N}\sum_{\mathbf{k},\omega_l}\frac{\varepsilon(\mathbf{k})\,\varepsilon(-\mathbf{k})Y_{\sigma,-\sigma}(i\omega_l)}{D_\sigma(\mathbf{k},i\omega_l)}$$

$$\times\,\bar{\mathcal{G}}_2^{(0)\,ir}(\sigma,i\omega;-\sigma,-i\omega|\sigma,i\omega_l;-\sigma,-i\omega_l). \tag{47}$$

In the same approximation Λ_σ has to be computed from

$$\Lambda_\sigma(i\omega) = \mathcal{G}_{p\sigma}^{(0)}(i\omega)$$

$$-\frac{1}{\beta N}\sum_{\mathbf{k},\omega_l}\frac{\varepsilon^2(\mathbf{k})}{D_\sigma(\mathbf{k},i\omega_l)}\{\Lambda_\sigma(i\omega_l)[1-\varepsilon(-\mathbf{k})\,\Lambda_{-\sigma}(-i\omega_l)]$$

$$-\,\varepsilon(\mathbf{k})\,Y_{\sigma,-\sigma}(i\omega_l)\,\bar{Y}_{-\sigma,\sigma}(i\omega_l)\}\,\bar{\mathcal{G}}_2^{(0)\,ir}(\sigma,i\omega;\sigma,i\omega_l|\sigma,i\omega_l;\sigma,i\omega)$$

$$-\frac{1}{\beta N}\sum_{\mathbf{k},\omega_l}\frac{\varepsilon^2(\mathbf{k})}{D_\sigma(\mathbf{k},i\omega_l)}\{\Lambda_{-\sigma}(-i\omega_l)[1-\varepsilon(\mathbf{k})\,\Lambda_\sigma(i\omega_l)]$$

$$-\,\varepsilon(-\mathbf{k})\,Y_{\sigma,-\sigma}(i\omega_l)\bar{Y}_{-\sigma,\sigma}(i\omega_l)\}\,\bar{\mathcal{G}}_2^{(0)\,ir}(\sigma,i\omega;-\sigma,i\omega_l|-\sigma,i\omega_l;\sigma,i\omega) \tag{48}$$

with

$$D_\sigma(\mathbf{k},i\omega) = [1-\varepsilon(\mathbf{k})\,\Lambda_\sigma(i\omega)][1-\varepsilon(-\mathbf{k})\,\Lambda_{-\sigma}(-i\omega)] + \varepsilon(\mathbf{k})\,\varepsilon(-\mathbf{k})\,Y_{\sigma,-\sigma}(i\omega)\,\bar{Y}_{-\sigma,\sigma}(i\omega). \tag{49}$$

The corresponding equation for $\bar{Y}_{-\sigma,\sigma}(i\omega)$ can be obtained from the expression for $Y_{\sigma,-\sigma}(i\omega)$.

The last equations together with the equations for the one- and two-particle Green's functions determine completely the properties of the superconducting phase, provided it exists. In order to gain further insight into the physics contained in (47) and (48) we will linearize the equations in terms of the order parameter $Y_{\sigma,-\sigma}(i\omega)$ which will determine the critical temperature T_c. The resulting equation for the order parameter is of the form

$$Y_{\sigma,-\sigma}(i\omega) = -\frac{1}{\beta N}\sum_{\mathbf{k},\omega_l}\frac{\varepsilon(\mathbf{k})\,\varepsilon(-\mathbf{k})Y_{\sigma,-\sigma}(i\omega_l)}{[1-\varepsilon(\mathbf{k})\,\Lambda_\sigma(i\omega_l)][1-\varepsilon(-\mathbf{k})\,\Lambda_{-\sigma}(-i\omega_l)]}$$

$$\times\,\bar{\mathcal{G}}_2^{(0)\,ir}(\sigma,i\omega;-\sigma,-i\omega|\sigma,i\omega_l;-\sigma,-i\omega_l). \tag{50}$$

This equation must be solved together with the equation for $\Lambda_\sigma(i\omega)$ which may be approxi-

mated by setting the order parameters to zero giving,

$$\Lambda_\sigma(i\omega) = \mathcal{G}_{p\sigma}^{(0)}(i\omega) - \frac{1}{\beta N} \sum_{\mathbf{k},\omega_l} \frac{\varepsilon^2(\mathbf{k})\,\Lambda_\sigma(i\omega_l)}{1 - \varepsilon(\mathbf{k})\,\Lambda_\sigma(i\omega_l)}\,\bar{\mathcal{G}}_2^{(0)\,ir}(\sigma, i\omega; \sigma, i\omega_l|\sigma, i\omega_l; \sigma, i\omega)$$

$$- \frac{1}{\beta N} \sum_{\mathbf{k},\omega_l} \frac{\varepsilon^2(\mathbf{k})\,\Lambda_{-\sigma}(i\omega_l)}{1 - \varepsilon(-\mathbf{k})\,\Lambda_{-\sigma}(i\omega_l)}\,\bar{\mathcal{G}}_2^{(0)\,ir}(\sigma, i\omega; -\sigma, i\omega_l| - \sigma, i\omega_l; \sigma, i\omega). \quad (51)$$

In order to determine T_c we must solve (51) for Λ_σ and insert the result in (50). The irreducible functions in (50) and (51) can be written as

$$\bar{\mathcal{G}}_2^{(0)\,ir}(\sigma, i\omega; \sigma, i\omega_l|\sigma, i\omega_l; \sigma, i\omega) = \frac{(\omega - \omega_l)^2}{\Delta^2\Delta_l^2}\Big\{2\omega_c^2(x + x_l)\tanh(\beta\epsilon/2)$$

$$- \frac{\coth(\beta\omega_c/2)}{\omega_c[(i\omega - i\omega_l)^2 - 4\omega_c^2]}\left[(xx_l + \omega_c^2)(\Delta\Delta_l + 8\omega_c^4) - 2\omega_c^2(\Delta + \Delta_l)(xx_l - \omega_c^2)\right]\Big\}, \quad (52)$$

$$\bar{\mathcal{G}}_2^{(0)\,ir}(\sigma, i\omega; -\sigma, i\omega_l| - \sigma, i\omega_l; \sigma, i\omega) = -\frac{2\omega_c}{\Delta^2\Delta_l^2}\Big\{\omega_c(x + x_l)(\Delta + \Delta_l)\tanh(\beta\epsilon/2)$$

$$+ \coth(\beta\omega_c/2)(x + x_l)^2(xx_l - \omega_c^2)\Big\} + \frac{\coth(\beta\omega_c/2)((xx_l + 3\omega_c^2)}{\omega_c\Delta\Delta_l}, \quad (53)$$

$$\bar{\mathcal{G}}_2^{(0)\,ir}(\sigma, i\omega; -\sigma, -i\omega|\sigma, i\omega_l; -\sigma, -i\omega_l) =$$

$$- \frac{2\epsilon(2\omega_c)^2\tanh(\beta\epsilon/2)[i\omega\,i\omega_l + \epsilon^2 - \omega_c^2]}{[\omega^2 + (\epsilon + \omega_c)^2][\omega^2 + (\epsilon - \omega_c)^2][\omega_l^2 + (\epsilon + \omega_c)^2][\omega_l^2 + (\epsilon - \omega_c)^2]}$$

$$+ \frac{2\omega_c\coth(\beta\omega_c/2)[i\omega\,i\omega_l + 2\omega_c(\epsilon - \omega_c) - (\epsilon - \omega_c)^2]}{[\omega^2 + (\epsilon - \omega_c)^2][\omega_l^2 + (\epsilon - \omega_c)^2][(\omega - \omega_l)^2 + (\epsilon + (2\omega_c)^2]}$$

$$+ \frac{2\omega_c\coth(\beta\omega_c/2)[i\omega\,i\omega_l - 2\omega_c(\epsilon + \omega_c) - (\epsilon + \omega_c)^2]}{[\omega^2 + (\epsilon + \omega_c)^2][\omega_l^2 + (\epsilon + \omega_c)^2][(\omega - \omega_l)^2 + (\epsilon + (2\omega_c)^2]}, \quad (54)$$

where

$$x = i\omega - \epsilon, \qquad\qquad \Delta = (i\omega - \epsilon)^2 - \omega_c^2 \qquad\qquad (55a)$$

$$x_l = i\omega_l - \epsilon, \qquad\qquad \Delta_l = (i\omega_l - \epsilon)^2 - \omega_c^2. \qquad\qquad (55b)$$

14

For further discussion of (50) and (51) we introduce the following shorthand notation:

$$\phi_\sigma(i\omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{\varepsilon^2(\mathbf{k})\, \Lambda_\sigma(i\omega)}{1 - \varepsilon(\mathbf{k})\, \Lambda_\sigma(i\omega)}$$

$$= \frac{1}{N} \sum_{\mathbf{k}} \frac{\varepsilon(\mathbf{k})}{1 - \varepsilon(\mathbf{k})\, \Lambda_\sigma(i\omega)}, \tag{56}$$

$$g_\sigma(i\omega) = \mathcal{G}(\mathbf{x} = \mathbf{x}'|i\omega)$$

$$= \frac{1}{N} \sum_{\mathbf{k}} \frac{\Lambda_\sigma(i\omega)}{1 - \varepsilon(\mathbf{k})\, \Lambda_\sigma(i\omega)}, \tag{57}$$

$$\phi_\sigma^{sc}(i\omega) = \frac{1}{N} \sum_{\mathbf{k}} \frac{\varepsilon(\mathbf{k})\, \varepsilon(-\mathbf{k})}{[1 - \varepsilon(\mathbf{k})\, \Lambda_\sigma(i\omega)][1 - \varepsilon(-\mathbf{k})\, \Lambda_{-\sigma}(-i\omega)]}$$

$$= \frac{\phi_\sigma(i\omega) - \phi_{-\sigma}(-i\omega)}{\Lambda_\sigma(i\omega) - \Lambda_{-\sigma}(-i\omega)}. \tag{58}$$

Furthermore we assume that $\varepsilon(\mathbf{k}) = \varepsilon(-\mathbf{k})$ holds with $\sum_{\mathbf{k}} \varepsilon(\mathbf{k}) = \sum_{\mathbf{k}} \varepsilon^3(\mathbf{k}) = 0$. Sums will be replaced by integrals,

$$\frac{1}{N} \sum_{\mathbf{k}} = \int d\varepsilon\, \rho_0(\varepsilon), \tag{59}$$

$$\rho_0(\varepsilon) = \frac{4}{\pi W} \sqrt{1 - \left(\frac{2\varepsilon}{W}\right)^2} \times \begin{cases} 1 & |\varepsilon| < \frac{W}{2}, \\ 0 & |\varepsilon| < \frac{W}{2}, \end{cases} \tag{60}$$

where W is the band width and ρ_0 a model density of states of semielliptic form. Since we do not consider magnetic states here, the spin index in the paramagnetic phase can be omitted:

$$\Lambda_\sigma(i\omega) = \Lambda_{-\sigma}(i\omega) = \Lambda(i\omega), \tag{61a}$$

$$\phi_\sigma(i\omega) = \phi_{-\sigma}(i\omega) = \phi(i\omega), \tag{61b}$$

$$\phi_\sigma^{sc}(i\omega) = \phi_{-\sigma}^{sc}(i\omega) = \phi^{sc}(i\omega). \tag{61c}$$

However, the spin index is essential for the superconducting order parameter $Y_{\sigma,-\sigma}(i\omega)$,

$$Y_{\sigma,-\sigma}(i\omega) = g_{\sigma,-\sigma} Y(i\omega), \tag{62a}$$

$$g_{\sigma,-\sigma} = \delta_{\sigma,\uparrow} - \delta_{\sigma,\downarrow}, \tag{62b}$$

where $Y(i\omega)$ is an even function of the frequency,

$$Y(i\omega) = Y(-i\omega). \tag{63}$$

15

Finally we have to add the equation which determines the chemical potential:

$$\frac{1}{\beta} \sum_{\omega_n} \sum_{\sigma} \mathcal{G}_\sigma(\mathbf{x} = \mathbf{x}'|i\omega) \, e^{i\omega_n 0^+} = \frac{2}{\beta} \sum_{\omega_n} g_\sigma(i\omega) \, e^{i\omega_n 0^+} = \frac{N_p}{N}. \tag{64}$$

Here N_p is the number of polarons and N the number of lattice sites. With (59) and (60) the functions (56) and (57) can be written as

$$\phi(i\omega) = \frac{W}{2} \frac{\left(1 - \sqrt{1 - \lambda^2(i\omega)}\right)^2}{\lambda^3(i\omega)} = \frac{W}{2} \frac{\lambda(i\omega)}{\left(1 + \sqrt{1 - \lambda^2(i\omega)}\right)^2} \tag{65}$$

$$g(i\omega) = \frac{4}{W} \frac{\left(1 - \sqrt{1 - \lambda^2(i\omega)}\right)^2}{\lambda(i\omega)} = \frac{4}{W} \frac{\lambda(i\omega)}{\left(1 + \sqrt{1 - \lambda^2(i\omega)}\right)^2}, \tag{66}$$

with $\lambda(i\omega) = (W/2)\,\Lambda(i\omega)$. In order to check whether the state to be determined from Eq. (51) is metallic or dielectric one has to analyze the renormalized density of states given by

$$\rho(E) = -\frac{1}{\pi} \operatorname{Im} g(E + i0^+) = -\frac{1}{\pi} \operatorname{Im} \left(\frac{1 - \sqrt{1 - \lambda^2(E + i0^+)}}{\lambda(E + i0^+)} \right), \tag{67}$$

where $\lambda(E + i0^+)$ is the analytical continuation of $\lambda(i\omega)$.

VI. ANALYTICAL SOLUTIONS

The expressions for $\Lambda(i\omega)$ and $Y(i\omega)$ simplify by using the shorthand notations (56) and (57) and the symmetry property (62):

$$Y(i\omega) = \frac{1}{\beta} \sum_{\omega_l} \phi^{sc}(i\omega_l) \, \bar{\mathcal{G}}^{(0)\,ir}(\sigma, i\omega; -\sigma, -i\omega|\sigma, i\omega_l; -\sigma, -i\omega_l) Y(i\omega_l), \tag{68}$$

$$\Lambda(i\omega) = \mathcal{G}_p^{(0)}(i\omega) - \frac{1}{\beta} \sum_{\omega_l} \phi(i\omega_l) \left[\bar{\mathcal{G}}^{(0)\,ir}(\sigma, i\omega; \sigma, i\omega_l|\sigma, i\omega_l; \sigma, i\omega) \right.$$

$$\left. + \bar{\mathcal{G}}^{(0)\,ir}(\sigma, i\omega; -\sigma, i\omega_l| -\sigma, i\omega_l; \sigma, i\omega) \right]. \tag{69}$$

In order to find a solution of Eq. (68) we insert (54), replace $Y(i\omega_n)$ by

$$Y(i\omega_n) = \phi^{sc}(z_0) \, \chi(i\omega_n) \, Y(z_0) \quad \text{with } z \simeq 0, \tag{70}$$

$$\chi(i\omega_n) = \frac{1}{\beta} \sum_{\omega_l} \bar{\mathcal{G}}^{(0)\,ir}(\sigma, i\omega_n; -\sigma, -i\omega_n|\sigma, i\omega_l; -\sigma, -i\omega_l)$$

$$= \frac{2\omega_c[\omega_c - \epsilon \tanh(\beta\epsilon/2) \cosh(\beta\omega_c/2)] + \cosh(\beta\omega_c)(-\omega_c^2 + \epsilon^2 + \omega_n^2)(\cosh(\beta\omega_c) - 1)^{-1}}{[\omega_n^2 + (\omega_c + \epsilon)^2][\omega_n^2 + (\omega_c + \epsilon)^2]}.$$

$$\tag{71}$$

and make use of Poisson's sum rule,

$$\frac{1}{\beta} \sum_{\omega_n} f(i\omega_n) = -\frac{1}{2\pi i} \int_C dz \, \frac{f(z)}{e^{\beta z} + 1}, \tag{72}$$

where C denotes the usual counterclockwise contour of the imaginary axis. We obtain then from Eq. (68) with help of the analytically continued function $\chi(z)$ for $Z = Z_0 = 0$ an equation for the critical temperature T_c,

$$\chi(0|\epsilon) \, \phi^{sc}(0|\epsilon) = 1, \tag{73}$$

$$\chi(0|\epsilon) = \left(2\omega_c[\omega_c - \epsilon \tanh(\beta_c \epsilon/2) \coth(\beta_c \omega_c/2)] + \frac{(\epsilon^2 - \omega_c^2) \cosh(\beta_c \omega_c)}{\cosh(\beta_c \omega_c) - 1}\right) \left(\omega_c^2 - \epsilon^2\right)^{-2}. \tag{74}$$

This quantity is even in ϵ and therefore only the absolute value of $\epsilon = \bar{\epsilon}_0 - \bar{\mu}$ determines $k_B T_c = \beta_c^{-1}$. From (58) and (65) one can make a rough guess for the quantity $\phi^{sc}(0)$:

$$\phi^{sc}(0) \approx \left(\frac{W}{4}\right)^2 \frac{1}{\gamma^2}, \quad \gamma = \frac{1}{2}\left(1 + \sqrt{1 - \lambda^2(0 + i\delta)}\right), \tag{75}$$

where γ has to satisfy: $\gamma(-\epsilon) = \gamma(\epsilon)$. This quantity can be obtained self-consistently from Eq. (64) for the chemical potential. For simplicity we replace here $[1 + \sqrt{1 - \lambda^2(0 + i\delta)}]$ by 2γ. Then (64) can be written as

$$\frac{2}{\gamma} \frac{1}{\beta} \sum_{\omega_n} \Lambda(i\omega_n) \, e^{i\omega_n 0^+} = \frac{N_p}{N}. \tag{76}$$

Using (69) together with (52) and (53) we can express $\Lambda(i\omega_n)$ as

$$\Lambda(i\omega_n) = \frac{(i\omega_n - \epsilon)A_1(\epsilon) + \omega_c B_1(\epsilon)}{(i\omega_n - \epsilon)^2 - \omega_c^2} + \frac{\omega_c^2[(i\omega_n - \epsilon)A_2(\epsilon) + \omega_c B_2(\epsilon)]}{[(i\omega_n - \epsilon)^2 - \omega_c^2]^2} \tag{77}$$

with unknown coefficients A_i and B_i. They can be found from Eq. (69) or more easily from the asymptotic behavior of (77) for $|\omega_n| \to \infty$,

$$\Lambda(i\omega_n) \underset{|\omega_n| \to \infty}{=} \frac{A_1}{i\omega_n} + \frac{A_1\epsilon + \omega_c B_1}{(i\omega_n)^2} + \frac{A_1(\omega_c^2 + \epsilon^2) + 2\epsilon\omega_c B_1 + \omega_c^2 A_2}{(i\omega_n)^3}$$
$$+ \frac{A_1(\epsilon^3 + 3\epsilon\omega_c^2) + B_1(\omega_c^3 + 3\epsilon^2\omega_c) + \omega_c^2(3\epsilon A_2 + \omega_c B_2)}{(i\omega_n)^4} + \dots \tag{78}$$

17

If we compare this with the asymptotic behavior of the full one-polaron Green's function (Appendix A) by invoking the methods of moments together with the asymptotic behavior of $g(i\omega_n)$ in (66), we obtain

$$A_1(\epsilon) = 1, \tag{79a}$$

$$B_1(\epsilon) = -\frac{1}{\omega_c}[M_1 + \epsilon], \tag{79b}$$

$$A_2(\epsilon) = \frac{1}{\omega_c^2}\left[M_2 + 2\epsilon M_1 + \epsilon^2 - \omega_c^2 - (W/4)^2\right], \tag{79c}$$

$$B_2(\epsilon) = \frac{1}{\omega_c^3}\left[-M_3 - 3\epsilon M_2 + M_1\left(\omega_c^2 - 3\epsilon^2 + 3(W/4)^2\right) + \epsilon\omega_c^2 - \epsilon^3 + 3\epsilon(W/4)^2\right], \tag{79d}$$

where M_i is the i-th moment of the one-polaron Green's function. The results in (A.5) for the moments in lowest order allow to evaluate A_i and B_i, see (A.7). $A_1 = 1$ describes the asymptotic freedom of the polarons. $B_1 = \tanh(\beta\epsilon/2)$ is identical with its value in the zero-order polaron Green's function of (38). The two new quantities A_2 and B_2 are small quantities being proportional to $\omega_0/\omega_c = 1/\alpha$

Inserting now (77) into the left-hand part of Eq. (76) and performing the summation leads to

$$\frac{1}{\beta}\sum_{\omega_n}\Lambda(i\omega_n)\,e^{i\omega_n 0^+} = \bar{n}(\epsilon)$$

$$+ \frac{\tanh(\beta\epsilon/2)\left[\tanh(\beta\omega_c/2) - 1\right]\left[1 - \tanh^2(\beta\epsilon/2)\right]}{2\left[1 - \tanh^2(\beta\omega_c/2)\tanh^2(\beta\epsilon/2)\right]}$$

$$+ \frac{B_2(\epsilon)}{4}\tanh(\beta\omega_c/2)\frac{1 - \tanh^2(\beta\epsilon/2)}{1 - \tanh^2(\beta\epsilon/2)\tanh^2(\beta\omega_c/2)}$$

$$- \frac{\beta\omega_c}{16}\left[\frac{A_2(\epsilon) + B_2(\epsilon)}{\cosh^2[\beta(\omega_c + \epsilon)/2]} - \frac{A_2(\epsilon) - B_2(\epsilon)}{\cosh^2[\beta(\omega_c - \epsilon)/2]}\right], \tag{80}$$

which, according to Eq. (76), is equal to $(\gamma/2)(N_p/N)$. Because of the large collective frequency, $\beta\omega_c \gg 1$, we may omit exponentially small quantities like $\exp(-\beta\omega_c)$. Since we are interested in results for electron numbers which are close to half filling ($\epsilon = 0$), also $|\epsilon| \ll \omega_c$ holds. Furthermore we will neglect contributions of the order $1/\alpha$. Then the equation for the chemical potential (74) is simply

$$\bar{n}(\epsilon) = \gamma n_p/2, \quad n_p = N_p/N. \tag{81}$$

If furthermore we use $\gamma = 1$ (free polarons) we obtain with (75) for $\phi^{sc}(0)$ the value

$$\phi^{sc}(0 = (W/4)^2 \tag{82}$$

18

which allows to write the equation for the critical temperature T_c in the following form

$$\epsilon^2 + \omega_c^2 - 2\epsilon\omega_c \tanh(\beta\epsilon/2) = (\omega_c^2 - \epsilon^2)^2 (4/W)^2. \tag{83}$$

In this approximation T_c depends only on the local parameters; but we expect that close to half filling this should give an impression which of the local quantities is most important for superconductivity in the strong-coupling limit of the Hubbard-Holstein model. For strictly half filling Eq. (83) can only be fulfilled when $\omega_c = W/4$. This may perhaps be an unphysical large value for the renormalized quantity. It also shows that the specific limit $\bar{U} = 0$ is probably the critical value for the occurence of superconductivity in the frame of the Hubbard-Holstein model. It is clear that for $\bar{U} < 0$ superconductivity is possible; but in this case it would have to compete in energy with the energies of charge-ordered states.

For the special case $\omega_c = W/4$ we obtain

$$(\epsilon/\omega_c)^2 \left[3 - (\epsilon/\omega_c)^2\right] = (2|\epsilon|/\omega_c) \tanh(\beta_c|\epsilon|/2). \tag{84}$$

Since $(\epsilon/\omega_c < 3$ holds (not discussed in detail) we may seek for solutions for the case $|\epsilon| \ll \omega_c$ leading to

$$k_B T_c = \frac{\omega_c}{3} \left[1 - \frac{5}{12}\left(\frac{\epsilon}{\omega_c}\right)^2 + \dots\right]$$
$$= \frac{W}{12} \left[1 - \frac{20}{3}\left(\frac{\epsilon}{W}\right)^2 + \dots\right]. \tag{85}$$

In spite of the many approximations (which however are all reasonable) used the result for T_c is in so far remarkable as it shows that the critical temperature depends on the band width (corresponding to the largest cut-off energy of the model) and not on the effective mass of the ions. for small deviations from half filling T_c decreases and does not depend on the sign of ϵ.

For different values of ω_c,

$$\omega_c = W/4 - y, \tag{86}$$

with $y \neq 0$ there are only solutions for not half filling. In this case Eq. (84) may in this case be written as

$$\beta_c|\epsilon| = \ln\frac{1+\kappa}{1-\kappa}, \tag{87}$$
$$\kappa = \frac{\epsilon^2 + \omega_c^2 - (4/W)^2(\omega_c^2 - \epsilon^2)^2}{2|\epsilon|\omega_c}, \quad 0 < \kappa < 1. \tag{88}$$

19

The condition $\kappa < 1$ is equivalent to

$$|\epsilon| + \omega_c < W/4 \tag{89}$$

while $\kappa > 0$ is related to the parameter y,

$$\omega_c < W/4, \ y > 0 : \quad (W/4 - \omega_c)^2 < \epsilon^2 < \epsilon_{\max}^2, \tag{90}$$

$$\omega_c > W/4, \ y < 0 : \quad \epsilon_{min}^2 < \epsilon^2 < \epsilon_{max}^2, \tag{91}$$

$$\epsilon_{max,\,min}^2 = \omega_c^2 + (1/2)(W/4)^2 \pm (W/8)\sqrt{(W/4)^2 + 8\omega_c^2}. \tag{92}$$

For small y we can simplify (87) and (88),

$$\kappa \simeq 2/(W|\epsilon|) \left\{ \epsilon^2[3 - \epsilon^2(4/W)^2] + y[W/2 - 4\epsilon^2/W - \epsilon^4(4(W)^3] \right.$$
$$\left. + y^2[-3 + \epsilon^2(4/W)^2 - \epsilon^4(4/W)^4], \right\} \tag{93}$$

with the following restrictions for ϵ:

$$y > 0 : \quad y^2 < \epsilon^2 < 3(W/4)^2 - (5/6)Wy + (29/27)y^2, \tag{94}$$

$$y < 0 : \quad (W/6)|y| + (25/27)y^2 < \epsilon^2 < 3(W/4)^2 + (5/6)W|y| + (29/27)y^2. \tag{95}$$

Large values for T_c can be achieved for $\kappa \lnsim 1$ and in the vicinity of half filling ($\epsilon \neq 0$):

$$k_B T_c \simeq \frac{W\delta}{12(\delta - 1)}, \quad \delta = \frac{6\epsilon^2}{W|y|} < 1, \quad y = \frac{W}{4} - \omega_c, \tag{96}$$

but only for $y < 0$ and hence $\omega_c > W/4$.

VII. SUMMARY

We have discussed the occurence of superconductivity for the Hubbard-Holstein model in the strong-coupling limit ($\bar{g} \gg 1$). Strong coupling leads to a renormalization of the one-polaron Green's function already in the local approximation. For $\bar{g} \gg 1$ we find a collective mode for the phonon clouds estimated by evaluating integrals in the Laplace approximation. Due to the absorption and emission of this mode by the polarons, the on-site energies of polarons are renormalized. Similarly the irreducible two-particle Green's are renormalized. Allowing for the exchange of polarons including their phonon clouds leads to a new irreducible Green's function which has been used to study spin-singlet pairing of polarons.

Analytical results for the superconducting phase have been obtained for the limiting case, for which the local repulsion of polarons is exactly canceled by their attractive interaction. The resulting equation for the critical temperature has been obtained by assuming a large collective-mode frequency and a nearly half-filled band case. The parameters which determine T_c are ω_c ($\geq W/4$), ϵ ($\epsilon = 0$ corresponds to half filling) and the band width W with T_c. In the strong-coupling limit we obtain a critical temperature which is of the order of $W/12$.

Acknowledgments

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APPENDIX A: METHOD OF MOMENTS

By using the Heisenberg representation of the one-polaron Green' function

$$\mathcal{G}_\sigma(\mathbf{x} - \mathbf{x}'|\tau - \tau') = \langle T\, \hat{c}_{\mathbf{x}\sigma}(\tau)\, \hat{\bar{c}}_{\mathbf{x}'\sigma'}(\tau') \rangle_H, \tag{A1}$$

with

$$\hat{c}_{\mathbf{x}\sigma}(\tau) = e^{\mathcal{H}\tau} c_{\mathbf{x}\sigma}\, e^{-\mathcal{H}\tau}, \tag{A2a}$$

$$\hat{\bar{c}}_{\mathbf{x}\sigma}(\tau) = e^{\mathcal{H}\tau} c_{\mathbf{x}\sigma}^\dagger\, e^{-\mathcal{H}\tau}, \tag{A2b}$$

we can write the asimptotic expansion of the Fourier representation (25) for $|\omega_n| \to \infty$ as

$$\mathcal{G}_\sigma(\mathbf{x} = 0|i\omega_n) = g_\sigma(i\omega_n) = \frac{1}{i\omega_n} - \frac{M_1}{(i\omega_n)^2} + \frac{M_2}{(i\omega_n)^3} - \frac{M_3}{(i\omega_n)^4} + \dots, \tag{A3}$$

$$M_n = \langle \{ c_{\mathbf{x}\sigma}^\dagger, \underbrace{[\mathcal{H}[\mathcal{H}\dots[\mathcal{H}, c_{\mathbf{x}\sigma}]\dots\dots]}_{n} \} \rangle_H. \tag{A4}$$

Here the statistical average $\langle\ldots\rangle_H$ is defined with respect to the full density matrix of the grand canonical ensemble. In the simplest approximation we obtain for the first three moments of the Green's functions the relations,

$$M_1 = -(\epsilon + \omega_c \tanh(\beta\epsilon/2), \tag{A5a}$$

$$M_2 = \epsilon^2 + \omega_c^2 + (W/4)^2 + 2\epsilon\omega_c \tanh(\beta\epsilon/2) + \omega_0\omega_c \coth(\beta\omega_c/2), \tag{A5b}$$

$$M_3 = -\{\epsilon^3 + 3\epsilon[\omega_c^2 + \omega_c\omega_0 \coth(\beta\omega_c/2) + (W/4)^2]$$
$$+ \omega_c \tanh(\beta\epsilon/2)\,[\,3\epsilon^2 + 3(W/4)^2 + \omega_c^2 + \omega_0^2 + 3\omega_0\omega_c \coth(\beta\omega_0/2)\,]\}. \tag{A5c}$$

The expressions for the moments can be used to determine the unknown coefficients, $A_n(\epsilon)$ $A_n(\epsilon)$, in the relation for $\Lambda_\sigma(i\omega)$, see Eq. (78), by considering also the asymptotic behavior of $g_\sigma(i\omega)$ in (66) for small values of $\lambda_\sigma(i\omega)$,

$$g_\sigma(i\omega) = (2/W)\lambda_\sigma(i\omega)\,[\,1 + (\lambda^2/4) + 2(\lambda^2/4)^2 + \ldots\,]. \tag{A6}$$

We then insert the asymptotic form for $\lambda_\sigma(i\omega)$ from (78). Comparing the corresponding equations fixes the coefficients $A_n(\epsilon)$ and $A_n(\epsilon)$,

$$A_1(\epsilon) = 1, \tag{A7a}$$

$$B_1(\epsilon) = -\frac{1}{\omega_c}[M_1 + \epsilon], \simeq \tanh(\beta\epsilon/2), \tag{A7b}$$

$$A_2(\epsilon) = \frac{1}{\omega_c^2}\left[M_2 + 2\epsilon M_1 + \epsilon^2 - \omega_c^2 - (W/4)^2\right] \simeq \frac{\omega_0}{\omega_c}\coth(\beta\omega/2), \tag{A7c}$$

$$B_2(\epsilon) = \frac{1}{\omega_c^3}\left[-M_3 - 3\epsilon M_2 + M_1\left(\omega_c^2 - 3\epsilon^2 + 3(W/4)^2\right) + \epsilon\omega_c^2 - \epsilon^3 + 3\epsilon(W/4)^2\right]$$
$$\simeq \frac{\omega_0}{\omega_c}\tanh(\beta\epsilon/2)\left[\frac{\omega_0}{\omega_c} + 3\coth(\beta\omega_0/2)\right]. \tag{A7d}$$

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